The Radially Vibrating Spherical Quantum Billiard

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Abstract

We consider the radially vibrating spherical quantum billiard as a representative example of vibrating quantum billiards. We derive necessary conditions for quantum chaos in d-term superposition states. These conditions are symmetry relations corresponding to the relative quantum numbers of eigenstates considered pairwise. In this discussion, we give special attention to eigenstates with null angular momentum (for which the aforementioned conditions are automatically satisfied). When these necessary conditions are met, we observe numerically that there always exist parameter values for which the billiard behaves chaotically. We focus our numerical studies on the ground and first excited states of the radially vibrating spherical quantum billiard with null angular momentum eigenstates. We observe chaotic behavior in this configuration and thereby dispel the common belief that one must pass to the semiclassical ($\hbar \longrightarrow 0$) or high quantum number limits in order to meaningfully discuss quantum chaos. The results in the present paper are also of practical import, as the radially vibrating spherical quantum billiard may be used as a model for the quantum dot nanostructure, the Fermi accelerating sphere, and intra-nuclear particle behavior.

1 Introduction

There has been considerable research in the last twenty years that seeks to marry quantum mechanics and dynamical systems theory into a coherent whole.[4, 6] In particular, the concept of quantum chaos extends the notions of classical Hamil-

tonian chaos to the quantum regime. There are three types of quantum chaotic behavior: "quantized chaos" ("quantum chaology"), "semiquantum chaos," and genuine "quantum chaos." Quantum chaology concerns the quantum structure of classically chaotic systems, semiquantum chaos refers to the chaotic dynamics of coupled classical and quantum systems, and genuine quantum chaos refers to chaotic dynamics of fully quantum systems.[3] No example of the third type of quantum chaos has been established, so the existence of such systems is an open question.

In the present paper, we discuss semiquantum chaos in the context of vibrating billiard systems. We review the recent results of Liboff and Porter[9] and discuss them in further detail. We treat a two-term Galërkin projection (superposition state) of the radially vibrating sphere and prove that only 2-term superpositions whose normal modes have common rotational symmetry behave chaotically. We extend this theorem to arbitrary superposition states by applying it pairwise. In the proof of this theorem, we establish integrable (non-chaotic) behavior by showing that the evolution equations reduce to a two-dimensional autonomous dynamical system, whose non-chaotic properties are known.[12] We then discuss two examples: one integrable superposition and one chaotic one. We compute Poincaré maps and thereby reveal chaotic characteristics such as regions of ergodicity and KAM islands.

We also discuss the present results with respect to the phenomenology of quantum chaos. The chaotic behavior in the radius a and conjugate momentum P corresponds to classical Hamiltonian chaos. The normal modes ψ_{nlm} depend on the radius, so they exhibit quantum-mechanical wave chaos. We also observe chaos in the Bloch variables (x, y, z), which correspond to quantum-mechanical probabilities. The dynamical equations describing the present system correspond to a two degree-of-freedom (*dof*) Hamiltonian system, where one degree-of-freedom is classical (corresponding to the so-called one "degree-of-vibration" (*dov*) radial motion) and one is quantum-mechanical (corresponding to the coupling coefficient μ). By coupling a single classical *dof* (which is necessarily integrable) with a single quantum *dof* (which must also be integrable), we obtain a genuinely chaotic system that provides an example of semiquantum chaos since it consists of a classical system coupled to a quantum one. We remark that we do not need to pass to the semiclassical ($\hbar \longrightarrow 0$) or high quantum number limits in order to observe chaos, as is commonly considered requisite for a meaningful analysis of quantum chaos.[6]

The radially vibrating spherical quantum billiard has several practical applications that complement its theoretical import. The most important one is that it may be used as a model for the quantum dot nanostructure.[10] At low temperatures, this microdevice component experiences vibrations due to zero-point motions, and at higher temperatures, it exhibits vibrations due to natural fluctuations. Another application is that the radially vibrating spherical quantum billiard generalizes Fermi's "bouncing-ball model" of cosmic ray acceleration.[1] Additionally, the radially vibrating spherical quantum billiard models the intradynamics of the nucleus, as the 'liquid drop' and 'collective' models of the nucleus include boundary vibrations. Consequently, the importance of the ra-

dially vibrating spherical quantum billiard lies not only in its expansion of the theory of quantum chaos but also in its applicability to problems in nuclear, atomic, and mesoscopic physics.

2 Statement of the Problem

The spherical quantum billiard addresses the quantum dynamics of a particle of mass m_0 confined to the interior of a spherical cavity of mass $M \gg m_0$ with smooth walls of radius a. The radius vibrates in an a priori unspecified manner, so that $a \equiv a(t)$. A two-component superposition state (Galërkin projection) of this quantum billiard is given using Dirac notation by

$$|\psi(r,\theta,\phi,t;a(t))\rangle = A_1(t)|nlm,t\rangle + A_2(t)|n'l'm',t\rangle, \tag{1}$$

where $A_1(t)$ and $A_2(t)$ are complex amplitudes. The numbers $\{n,l,m\}$ are, respectively, the principal, orbital, and azimuthal quantum numbers. The eigenstates of the present system are products of spherical Bessel functions and spherical harmonics.[8] In coordinate representation,

$$\langle\vec{r}|nlm,t\rangle = \psi_{nlm}(r,\theta,\phi,t;a(t)) = \sqrt{\frac{2}{a(t)^3}}\left(\frac{1}{j_{l+1}(x_{ln})}\right) j_l\left(\frac{r x_{ln}}{a(t)}\right) Y_{lm}(\theta,\phi), \tag{2}$$

where x_{ln} is the nth zero of j_l, the spherical Bessel function of order l.

For the system at hand, the time-dependent Schrödinger equation is given by

$$i\hbar\frac{\partial\psi}{\partial t} = K\psi, \qquad r \le a(t), \tag{3}$$

where the quantum-mechanical Hamiltonian K, the kinetic energy of the particle, is

$$K = -\frac{\hbar^2}{2m_0}\nabla^2. \tag{4}$$

The total Hamiltonian of the system is

$$H = \frac{P^2}{2M} + V + K, \tag{5}$$

where P is the momentum of the billiard boundary, and $V \equiv V(a)$ is the potential of the billiard surface. The potential energy V and kinetic energy $P^2/2M$ of the billiard walls are classical quantities, and the confined particle is quantum-mechanical. For this semiquantum system, we utilize the Born-Oppenheimer approximation[2], so that only the particle kinetic energy K is inserted into the Schrödinger equation (3). In this adiabatic approximation,

which is commonly used in mesoscopic physics, we are ignoring the effects of Berry phase.[13]

Taking the expectation of (3) using the superposition state (1) gives

$$\left\langle \psi \middle| -\frac{\hbar^2}{2m_0}\nabla^2\psi \right\rangle = \frac{1}{a^2}\left[\epsilon_1|A_1|^2 + \epsilon_2|A_2|^2\right] \equiv K(A_1, A_2, a),$$
$$i\hbar\left\langle \psi \middle| \frac{\partial\psi}{\partial t} \right\rangle = i\hbar\left[\dot{A}_1A_1^* + \dot{A}_2A_2^* + \nu_{11}|A_1|^2 + \nu_{12}A_1A_2^* + \nu_{21}A_2A_1^* + \nu_{22}|A_2|^2\right], \tag{6}$$

where the energies of the two terms are given by

$$\epsilon_1 \equiv \frac{\hbar^2 x_{ln}^2}{2m_0}, \qquad \epsilon_2 \equiv \frac{\hbar^2 x_{l'n'}^2}{2m_0}. \tag{7}$$

3 Integrable Configuration

Examining the superposition of $|100\rangle$ and $|110\rangle$ using (6) and orthogonality of spherical harmonics shows that $\nu_{11} = \nu_{12} = \nu_{21} = \nu_{22} = 0$. (Note that ν_{11} and ν_{22} vanish no matter which eigenstates one considers.) Equating the inner products (6) of both sides of the Schrödinger equation gives equations of motion for the complex amplitudes:

$$i\dot{A}_1 = \frac{1}{\hbar a^2}\epsilon_1 A_1, \qquad i\dot{A}_2 = \frac{1}{\hbar a^2}\epsilon_2 A_2, \tag{8}$$

which are integrated to yield

$$A_1(t) = C_1 \exp\left[-\frac{i\epsilon_1}{\hbar}\int a^{-2}(t)dt\right], \qquad A_2(t) = C_2 \exp\left[-\frac{i\epsilon_1}{\hbar}\int a^{-2}(t)dt\right]. \tag{9}$$

From (9), one obtains a Hamiltonian in the radius a and conjugate momentum P:

$$H = \frac{P^2}{2M} + K(A_1, A_2, a) + V(a) = \frac{P^2}{2M} + \frac{1}{a^2}\left[\epsilon_1|C_1|^2 + \epsilon_2|C_2|^2\right] + V(a). \tag{10}$$

A Hamiltonian with no explicit time-dependence and one *dof* corresponds to a two-dimensional autonomous system, which is known to be non-chaotic.[5, 12] When there are no coupling terms, the degree-of-freedom of the resulting Hamiltonian corresponds to the degree-of-vibration of the quantum billiard, which is a measure of the number of distance dimensions that undergo oscillations. When a two-term superposition has a non-vanishing coupling coefficient, the number of degrees-of-freedom of the resulting Hamiltonian system is equal to the number of *dov* of the billiard plus one. In particular, this means that a superposition state of a quantum billiard with more than one *dov* (such as the two *dov* rectangular quantum billiard) is expected to behave chaotically even if every one of its coupling coefficients vanishes.

Hamilton's equations for the present integrable configuration are

$$\dot{a} = \frac{P}{M} \equiv \frac{\partial H}{\partial P}, \qquad \dot{P} = -\frac{\partial V}{\partial a} + \frac{\lambda}{a^3} \equiv -\frac{\partial H}{\partial a}, \tag{11}$$

where the energy parameter λ is given by

$$\lambda \equiv 2\left(\epsilon_1 |C_1|^2 + \epsilon_1 |C_2|^2\right) > 0. \tag{12}$$

The bifurcation structure of (11) has been studied for quartic potentials $V(a)$.[11]

4 Necessary Conditions for Chaos in k Coupled States

Consider the superposition

$$\psi = A_1 \psi_{q_1} + A_2 \psi_{q_2} + \cdots + A_k \psi_{q_k}, \tag{13}$$

where $q_i \equiv (n_i, l_i, m_i)$ is a vector of quantum numbers. If there does not exist a pair of normal modes in the k-state superposition (13) with common angular momentum quantum numbers (i.e., there is no pair $\{i, i'\}$ such that $l_i = l_{i'}$ and $m_i = m_{i'}$), then inserting (13) into the Schrödinger equation (3) returns a diagonal quadratic form

$$\dot{A}_1 A_1^* + \cdots + \dot{A}_k A_k^* = \nu_{11} |A_1|^2 + \cdots + \nu_{kk} |A_k|^2, \tag{14}$$

as all the cross terms $\nu_{ij} A_i A_j^*$ have vanishing coupling coefficients ν_{ij} by orthogonality of spherical harmonics with different angular momenta. The diagonal terms in (14) stem from the Laplacian. As above, we obtain the Hamiltonian

$$H(a, P) = \frac{P^2}{2M} + \frac{1}{a^2} \sum_{i=1}^{k} \epsilon_i |C_i|^2 + V(a), \tag{15}$$

where the C_i are constants. The superposition (13) is non-chaotic, because the Hamiltonian (15) is autonomous with one *dof*.

We thus conclude that a necessary condition for chaotic behavior in an arbitrary finite superposition state of the radially vibrating spherical quantum billiard is that at least one pair of normal modes in the eigenfunction expansion have common angular momentum quantum numbers. In particular, by considering small n_i and $n_{i'}$, we obtain a chaotic superposition for eigenstates with small energies. This even holds for some superpositions that include the ground state! In most studies of quantum chaos, one must take the semiclassical ($\hbar \longrightarrow 0$) or high quantum-number limits in order to meaningfully study quantum chaos.[3, 6] In such studies, termed "quantum chaology," one considers the quantum signatures of classically chaotic systems in these regimes. In the present system, on the other hand, we obtain genuinely chaotic behavior in a semiquantum system. This phenomenon is often called "semiquantum chaos."[3]

5 Chaotic Configuration

As an example of a chaotic configuration of the radially vibrating spherical quantum billiard, consider the superposition state consisting of the ground and first excited states with null angular momentum

$$|\psi(n,l,m)\rangle = A_1|100\rangle + A_2|200\rangle, \tag{16}$$

which gives the wavefunction

$$\psi(r,t) = A_1(t)\alpha_1\psi_1(r,t)e^{-i\frac{E_1 t}{\hbar}} + A_2(t)\alpha_2\psi_2(r,t)e^{-i\frac{E_2 t}{\hbar}}, \tag{17}$$

where

$$\psi_n(r,t) = j_0\left(\frac{n\pi r}{a(t)}\right), \qquad j_0(x) = \frac{sin(x)}{x}, \qquad \alpha_n = \frac{\sqrt{2}}{a^{\frac{3}{2}} j_1(n\pi)}. \tag{18}$$

The superposition (16) has a coupling coefficient $\mu \equiv \mu_{12} = 4/3$.

Equating coefficients in the quadratic form (6) gives the matrix equation

$$i\dot{A}_n = \sum_{k=1}^{2} D_{nk}A_k, \tag{19}$$

where $D \equiv (D_{ij})$ is the Hermitian matrix

$$D = \begin{pmatrix} \frac{\epsilon_1}{\hbar a^2} & -i\mu\frac{\dot{a}}{a} \\ i\mu\frac{\dot{a}}{a} & \frac{\epsilon_2}{\hbar a^2} \end{pmatrix}, \tag{20}$$

and the energy coefficient ϵ_j is given by

$$\epsilon_j \equiv \frac{(j\pi\hbar)^2}{2m_0}, \qquad j \in \{1,2\}. \tag{21}$$

Defining the density matrix[8] by $\rho_{qn} = A_q A_n^*$, introducing (dimensionless) Bloch variables $x \equiv \rho_{12} + \rho_{21}$, $y \equiv i(\rho_{21} - \rho_{12})$, and $z \equiv \rho_{22} - \rho_{11}$, and using (19), we obtain the following three differential equations:

$$\dot{x} = -\frac{\omega_0 y}{a^2} - \frac{2\mu P z}{Ma}, \qquad \dot{y} = \frac{\omega_0 x}{a^2}, \qquad \dot{z} = \frac{2\mu P x}{Ma}. \tag{22}$$

In these equations, $\omega_0 \equiv (\epsilon_2 - \epsilon_1)/\hbar$. Rewriting the kinetic energy $K(A_1, A_2, a)$ in terms of the Bloch variable z gives

$$K(z,a) = \frac{1}{a^2}(\epsilon_+ + z\epsilon_-), \qquad \epsilon_\pm \equiv \frac{1}{2}(\epsilon_2 \pm \epsilon_1). \tag{23}$$

Inserting $K(z,a)$ into the Hamiltonian (5) gives Hamilton's equations:

$$\dot{a} = \frac{P}{M}, \qquad \dot{P} = -\frac{\partial V}{\partial a} + \frac{2}{a^3}\left[\epsilon_+ + \epsilon_-(z - \mu x)\right]. \tag{24}$$

Equations (22) and (24) constitute a set of five coupled nonlinear ordinary differential equations, which can be shown to be equivalent to a two degree-of-freedom Hamiltonian system. The constants of motion of the present system are the radius of the Bloch sphere

$$x^2 + y^2 + z^2 \equiv |A_1|^2 + |A_2|^2 = 1 \tag{25}$$

and the energy (total Hamiltonian)

$$H = \frac{P^2}{2M} + V(a) + K(z, a). \tag{26}$$

The equilibria of equations (22, 24) satisfy $x = y = 0$, $z = \pm 1$, $P = 0$, and $a = a_\pm$, where $a_\pm$ satisfies the equation

$$\frac{\partial V}{\partial a} = \frac{2}{a^3}(\epsilon_+ \pm \epsilon_-), \tag{27}$$

where the subscript of $a_\pm$ corresponds to the sign of $z = \pm 1$. Assuming that $V(a) + K(z, a)$ has a single minimum in a, these equilibria are elliptic.[9, 11] (That is, every eigenvalue of the Jacobian of the linearized system is purely imaginary.) For the harmonic potential

$$V(a) = \frac{V_0}{a_0^2}(a - a_0)^2, \tag{28}$$

the total energy of the billiard's boundary is given by

$$V(a) + K(a) = \frac{V_0}{a_0^2}(a - a_0)^2 + \frac{\epsilon_+ + z\epsilon_-}{a^2}. \tag{29}$$

With this choice of potential, equation (27) becomes

$$a - a_0 = \frac{a_0^2 \epsilon_\pm}{V_0 a^3}. \tag{30}$$

The solutions of (30) for the equilibrium radii $a_\pm$ correspond to the $\epsilon_\pm$ values. One computes that $a_+ \geq a_- \geq a_0$, from which it follows that $a_- \leq a(0) \leq a_+$, so $a(t)$ remains bounded in the interval $[a_-, a_+]$.[9]

Now consider the superposition of the first k null angular momentum eigenstates,

$$\psi^{(k)}(r) = \sum_{n=1}^{k} A_n(t)\alpha_n\psi_n(r, t). \tag{31}$$

In order to analyze this configuration, one first examines the 2-term superposition

$$\psi_{nq} = A_n(t)\alpha_n\psi_n(r, t) + A_q(t)\alpha_q\psi_q(r, t), \qquad n < q, \tag{32}$$

and then superposes the couplings one obtains from each ψ_{nq} as n and q run from 1 to k in order to obtain dynamical equations for the amplitudes A_i. One computes the coupling coefficients μ_{nq} to be

$$\mu_{nq} = 2\frac{qn}{a(t)(n+q)(q-n)}, \qquad n \neq q. \tag{33}$$

The dynamical equations for A_i are described by a $k \times k$ matrix and are a straightforward generalization of (19, 20).

5.1 Numerical simulations

The analysis for 2-term superpositions of null angular momentum eigenstates follows that for the general case.[9] In the present case, the necessary conditions for chaotic behavior are satisfied automatically, because the quantum numbers m and l vanish for every normal mode under consideration. Consequently, any k-term superposition ($k \geq 2$) of null angular momentum eigenstates exhibits chaotic behavior. We consider numerical simulations for the coupling of the ground state and first excited state of a billiard residing in a harmonic potential.

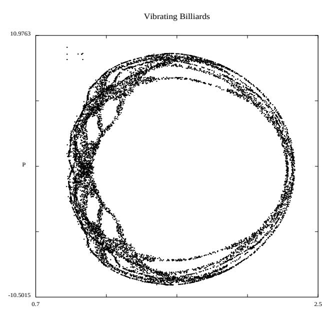

Figure 1: Poincaré Section ($x = 0$) in the (a, P)-plane illustrating that not all invariant tori are destroyed in the present configruation.

Figure 1 shows a Poincaré map in the (a, P)-plane corresponding to $x = 0$, and Figure 2 shows a Poincaré section projected onto the (x, y)-plane for $P = 0$. For each of these two plots, we used the parameter values $\hbar = 1$, $M = 10$, $m = 1$, $V_0/a_0^2 = 5$, and $a_0 = 1.25$. The initial conditions for the two figures are $x(0) = \sin(0.95\pi) \approx 0.156434$, $y(0) = 0$, $z(0) = \cos(0.95\pi) \approx -0.987688$, $a(0) \approx 1.6$, and $P(0) \approx 9.45$.

The chaotic behavior of this configuration is evident in both plots, although there is clearly still some non-chaotic structure present. In the language of KAM theory, some of the nonresonant tori persist for the present choice of initial conditions[5, 12]. One may also choose initial conditions corresponding to a different level of persistence of the resonant tori. For example, Figure 3 shows an $x = 0$ Poincaré map in the (a, P)-plane with the same initial conditions and parameter values as above, except $a(0) = 3$ and $P(0) = 10$. Figure 4 shows a $P = 0$ Poincaré map in the (x, y)-plane for these conditions. There are fewer invariant tori in these two figures than there are in Figures 1–2.

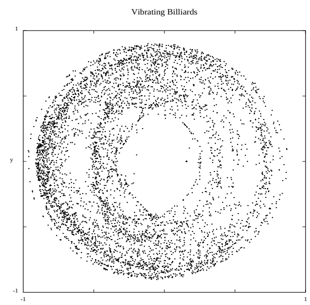

Figure 2: Poincaré Section ($P = 0$) of the Bloch sphere projected onto the (x, y)-plane. The structure in this diagram likewise illustrates the survival of some invariant tori.

6 Phenomenology

In contrast to the present quantum-mechanical context, we note that for the classical radially vibrating spherical billiard, every orbit with null angular momentum is well-defined and invariant under radial oscillations of the boundary.[7] Due to conservation of angular momentum, one finds that for the stationary spherical classical billiard, the enclosed particle sweeps out an annular domain of constant inner radius.[9] Vibration of the wall of the sphere destroys this constant, and chaotic motion is expected to develop. In the present quantum-mechanical context, we note that null angular momentum wavefunctions are composed only of spherical waves. The nodal surfaces of these wavefunctions are likewise spherical. Accordingly, the chaotic signature of this configuration in real space is the sequence of intersections with a fixed radius that nodal surfaces make at any instant subsequent to a number of transversal times.[9] This latter condition is consistent with the standard long-time behavior of chaotic dynamical systems.[6]

In the language of Blümel and Reinhardt[3], vibrating quantum billiards are an example of semiquantum chaos. One has a classical system (the walls of the billiard) coupled to a quantum-mechanical one (the enclosed particle). Considered individually, each of these subsystems is integrable, as each contributes a single *dof*. When they are coupled, however, one observes chaotic behavior in both of them. The classical variables (a, P) exhibit Hamiltonian chaos, whereas the quantum subsystem (x, y, z) is truly quantum chaotic. Chaos on the Bloch sphere is an example of quantum chaos because the Bloch variables (x, y, z) correspond to the quantum probabilities of the wavefunction. Additionally, each individual normal mode ψ_n depends on the radius $a(t)$, so each eigenfunction is an example of quantum-mechanical wave chaos for chaotic configurations of the billiard. Moreover, because the evolution of the probabilities $|A_i|^2$ is chaotic, the wavefunction ψ in the present configuration is a *chaotic combination* of chaotic

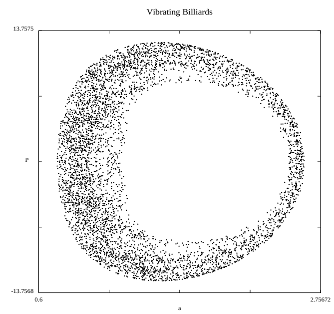

Figure 3: Poincaré Section ($x = 0$) in the (a, P)-plane for slightly different initial conditions in which fewer invariant tori persist. This is in accord with KAM theory.

normal modes. Finally, we note that if we quantize the motion of the billiard walls, we would obtain a higher-dimensional, fully-quantized system that exhibits so-called quantized chaos.[3] In particular, the fully quantized version of the present system would require passage to the semiclassical limit in order to observe quantum signatures of classical chaos.

7 Conclusions

We considered the radially vibrating spherical quantum billiard as a representative example of vibrating quantum billiards. We derived necessary conditions for quantum chaos in k-term superposition states. We gave special attention to eigenstates with null angular momentum, for which these conditions are automatically satisfied. We examined a numerical simulation of the superposition of the ground and first null angular momentum excited states. We observed chaotic behavior in this configuration, thereby dispelling the common belief that one is required to pass to the semiclassical ($\hbar \longrightarrow 0$) or high quantum number limits in order to meaningfully study quantum chaos.

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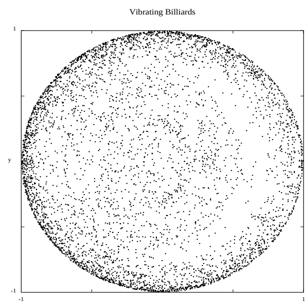

Figure 4: Poincaré Section ($P = 0$) of the Bloch sphere projected onto the (x, y)-plane. The initial conditions in this plot are the same as those in Figure 3.

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